PRML学习笔记——第五章

Neural Network

Feed-forward Network Functions

前面讨论的model的一般形式:

$$y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=1}^{M} w_j \phi_j(\mathbf{x})\right)$$

其中的ϕ是fix的basis function,如果考虑把basis function也引入parameter,这就是neural network.

$$y_k(\mathbf{x}, \mathbf{w}) = \sigma\left(\sum_{j=0}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right)\right)$$

这是两层network.

5.1.1 Weight-space symmetries

对于一个general network,同样的从input到output的mapping function可以用不同的$\mathbf{w}$来实现,这被称为weight-space symmetries.

5.2. Network Training

1. 对于regression,activation取identity function, loss取SSE.
2. 对于one-class classification,activation取一个logistic sigmoid output, loss取NLL(cross entropy).
3. 对于multiclass classification,activation取softmax, loss取multiclass cross entropy.

5.2.1 Parameter optimization

Neural network无法保证loss在参数空间上是convex的.满足$\nabla E(\mathbf{w}) = 0$的weight可能到达minimum,maximum,saddle points.因此一般来说只期望找到一个local minimum(并且general来说也无法知道是不是global minimum).

好在neural network是连续的,所以可以通过迭代的方法,每次更新搜索方向,得到一个较好的解.

5.2.2 Local quadratic approximation

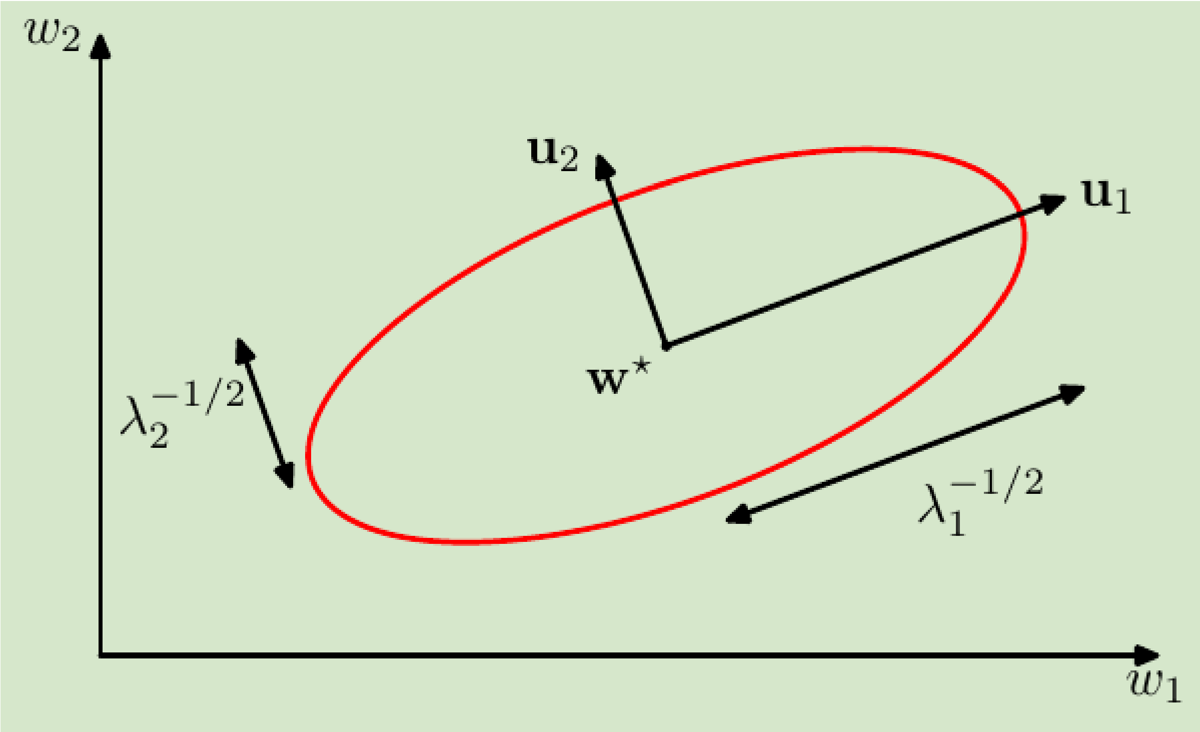
考虑$E(\mathbf{w})$在$\hat{\mathbf{w}}$的Taylor展开:

$$E(\mathbf{w}) \simeq E(\widehat{\mathbf{w}}) + (\mathbf{w} - \widehat{\mathbf{w}})^{\mathrm{T}} \mathbf{b} + \frac{1}{2}(\mathbf{w} - \widehat{\mathbf{w}})^{\mathrm{T}} \mathbf{H}(\mathbf{w} - \widehat{\mathbf{w}})$$

为了从几何上看,考虑$\mathbf{H}$的eigenvalue:

$$\mathbf{H}\mathbf{u}_i = \lambda_i \mathbf{u}_i$$

那么空间中任意一个$\mathbf{w}$ vector都可以表示成:$\mathbf{w} - \mathbf{w}^\star = \sum_i \alpha_i \mathbf{u}_i$,想当于先将坐标origin平移到$\mathbf{w}^\star$,然后再将坐标轴旋转align到每个$\mathbf{H}$的eigenvector.



那么:

$$E(\mathbf{w})=E\left(\mathbf{w}^{\star}\right)+\frac{1}{2}\sum_{i}\lambda_{i}\alpha_{i}^{2}$$

现在:$\mathbf{H}$正定 $\Longleftrightarrow$ 所有eigenvalue大于0 $\Longleftrightarrow$ $E(\mathbf{w}^{\star})$是local minimum.

5.2.3 Use of gradient information

不使用Gradient information,每次求minimum都需要$O\left(W^{3}\right)$.使用gradient information,可以降为$O\left(W^{2}\right)$.

5.2.4 Gradient descent optimization

Optimize neural network parameter的一个简单且有效的method就是gradient descent:

$$\mathbf{w}^{(\tau+1)}=\mathbf{w}^{(\tau)}-\eta\nabla E\left(\mathbf{w}^{(\tau)}\right)$$

当使用whole dataset 更新一次weight时被称为*batch* methods.

另一个版本是on-line 的gradient descent:

$$\mathbf{w}^{(\tau+1)}=\mathbf{w}^{(\tau)}-\eta\nabla E_{n}\left(\mathbf{w}^{(\tau)}\right)$$

也被称为sequential gradient descent/ stochastic gradient descent.好处是不仅更新快,并且容易跳出

local minimum.

5.3. Error Backpropagation

1. 首先输入input vector $\mathbf{x}_n$到network,并利用

$$a_j=\sum_i w_{ji} z_i$$

$$z_j=h\left(a_j\right).$$

   直到计算得到output
2. Evaluating δ_k for every **output** unit:

$$\delta_j \equiv \frac{\partial E_n}{\partial a_j}=\sum_k \frac{\partial E_n}{\partial a_k} \frac{\partial a_k}{\partial a_j}$$

3. backpropagate δ:

$$\delta_j=h^{\prime}\left(a_j\right) \sum_k w_{k j} \delta_k$$

4. 计算所有unit的gradient:

$$\frac{\partial E_n}{\partial w_{j i}}=\delta_j z_i$$

5.3.3 Efficiency of backpropagation

Backpropagation的复杂度是$O(W)$.考虑若用数值差分的方法替代:

$$\frac{\partial E_n}{\partial w_{j i}}=\frac{E_n\left(w_{j i}+\epsilon\right)-E_n\left(w_{j i}\right)}{\epsilon}+O(\epsilon)$$
$$\frac{\partial E_n}{\partial w_{j i}}=\frac{E_n\left(w_{j i}+\epsilon\right)-E_n\left(w_{j i}-\epsilon\right)}{2 \epsilon}+O\left(\epsilon^2\right)$$

由于对于每个weight都需要单独计算绕动,所以导致复杂度变成了$O(W^2)$.

5.3.4 The Jacobian matrix

Jacobian matrix同样可以通过反向传播来计算.

$$
\begin{aligned}
J_{ki} = \frac{\partial y_k}{\partial x_i} &= \sum_j \frac{\partial y_k}{\partial a_j} \frac{\partial a_j}{\partial x_i} \\
&= \sum_j w_{ji} \frac{\partial y_k}{\partial a_j}
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial y_k}{\partial a_j} &= \sum_l \frac{\partial y_k}{\partial a_l} \frac{\partial a_l}{\partial a_j} \\
&= h'\left(a_j\right) \sum_l w_{lj} \frac{\partial y_k}{\partial a_l}
\end{aligned}
$$

这样就能递归地得到结果.

5.4. The Hessian Matrix

5.4.1 Diagonal approximation

Hessian Matrix的element为:

$$
\frac{\partial^2 E}{\partial w_{ji} \partial w_{lk}}
$$

直接求解整个matrix的每个element复杂度是$O(W)$.当假设所有非对角元素为0时能简化计算到$O(W)$.
对每个对角元素:

$$
\frac{\partial^2 E_n}{\partial w_{ji}^2} = \frac{\partial^2 E_n}{\partial a_j^2} z_i^2
$$

利用链式微分法则:

$$
\frac{\partial^2 E_n}{\partial a_j^2} = h'(a_j)^2 \sum_k \sum_{k'} w_{kj} w_{k'j} \frac{\partial^2 E_n}{\partial a_k \partial a_{k'}} + h''\left(a_j\right) \sum_k w_{kj} \frac{\partial E^n}{\partial a_k}
$$

假设非对角元素都是0:

$$
\frac{\partial^2 E_n}{\partial a_j^2} = h'(a_j)^2 \sum_k w_{kj}^2 \frac{\partial^2 E_n}{\partial a_k^2} + h''\left(a_j\right) \sum_k w_{kj} \frac{\partial E_n}{\partial a_k}
$$

5.4.2 Outer product approximation

对于SSE的error function:

$$E=\frac{1}{2} \sum_{n=1}^{N}\left(y_{n}-t_{n}\right)^{2}$$

Hessian matrix可以写成:

$$\mathbf{H}=\nabla \nabla E=\sum_{n=1}^{N} \nabla y_{n} \nabla y_{n}+\sum_{n=1}^{N}\left(y_{n}-t_{n}\right) \nabla \nabla y_{n}$$

前面谈到过对于一个最优的Regression solution就是$\mathbb{E}[\mathbf{t} \mid \mathbf{x}]$.这也就意味着$\nabla \nabla y_{n}$项可以被忽略.所以:

$$\mathbf{H} \simeq \sum_{n=1}^{N} \mathbf{b}_{n} \mathbf{b}_{n}^{\mathrm{T}}$$

其中$\mathbf{b}_{n}=\nabla y_{n}=\nabla a_{n}$,因为activation就是identity.

对于Cross entropy error function和sigmoid activation来说:

$$\mathbf{H} \simeq \sum_{n=1}^{N} y_{n}\left(1-y_{n}\right) \mathbf{b}_{n} \mathbf{b}_{n}^{\mathrm{T}}$$

5.4.3 Inverse Hessian

因为$\mathbf{H}_{N}=\sum_{n=1}^{N} \mathbf{b}_{n} \mathbf{b}_{n}^{\mathrm{T}}$.我们可以sequential估计$\mathbf{H}$:

\mathbf{H}_{L+1}=\mathbf{H}_{L}+\mathbf{b}_{L+1} \mathbf{b}_{L+1}^{\mathrm{T}}

为了sequential估计Hessian的inverse,引入一个matrix identity:
\left(\mathbf{M}+\mathbf{v v}^{\mathrm{T}}\right)^{-1}=\mathbf{M}^{-1}-\frac{\left(\mathbf{M}^{-1} \mathbf{v}\right)\left(\mathbf{v}^{\mathrm{T}} \mathbf{M}^{-1}\right)}{1+\mathbf{v}^{\mathrm{T}} \mathbf{M}^{-1} \mathbf{v}}

那么:
\mathbf{H}_{L+1}^{-1}=\mathbf{H}_{L}^{-1}-\frac{\mathbf{H}_{L}^{-1} \mathbf{b}_{L+1} \mathbf{b}_{L+1}^{\mathrm{T}} \mathbf{H}_{L}^{-1}}{1+\mathbf{b}_{L+1}^{\mathrm{T}} \mathbf{H}_{L}^{-1} \mathbf{b}_{L+1}}

5.4.4 Finite differences

如果直接使用finite difference 来求出Hessian matrix:

$$\begin{array}{l} \frac{\partial^{2} E}{\partial w_{j i} \partial w_{l k}}=\frac{1}{4 \epsilon^{2}}\left\{E\left(w_{j i}+\epsilon, w_{l k}+\epsilon\right)-E\left(w_{j i}+\epsilon, w_{l k}-\epsilon\right)\right. \\ \left.-E\left(w_{j i}-\epsilon, w_{l k}+\epsilon\right)+E\left(w_{j i}-\epsilon, w_{l k}-\epsilon\right)\right\}+O\left(\epsilon^{2}\right) \end{array}$$

这里面一共O(W^2)元素,每个元素需要O(W)的operation,所以总的复杂度是O(W^3).

现在只在第二阶difference时使用一次central difference:

$$\frac{\partial^{2} E}{\partial w_{j i} \partial w_{l k}}=\frac{1}{2 \epsilon}\left\{\frac{\partial E}{\partial w_{j i}}\left(w_{l k}+\epsilon\right)-\frac{\partial E}{\partial w_{j i}}\left(w_{l k}-\epsilon\right)\right\}+O\left(\epsilon^{2}\right)$$

现在只需要perturbe一共O(W)个weight,从而总的开销是O(W^2)

5.4.5 Exact evaluation of the Hessian

记:

$$\delta_{k}=\frac{\partial E_{n}}{\partial a_{k}}, \quad M_{k k^{\prime}} \equiv \frac{\partial^{2} E_{n}}{\partial a_{k} \partial a_{k^{\prime}}}$$

Hessian matrix可以精确的计算得到,考虑以最简单的一层hidden layer为例.

$$\frac{\partial^{2} E_{n}}{\partial w_{j i}^{(1)} \partial w_{k j^{\prime}}^{(2)}}=x_{i} h^{\prime}\left(a_{j^{\prime}}\right)\left\{\delta_{k} I_{j j^{\prime}}+z_{j} \sum_{k^{\prime}} w_{k^{\prime} j^{\prime}}^{(2)} H_{k k^{\prime}}\right\}$$

5.4.6 Fast multiplication by the Hessian

有时候计算Hessian的目的只是为了得到$\mathbf{v}^\mathrm{T}\mathbf{H}$的结果.也就是只需要O(W)的storage.如此跳过计算Hessian这个中间步骤更加高效.

Take note:

$$\mathbf{v}^{\mathrm{T}} \mathbf{H}=\mathbf{v}^{\mathrm{T}} \nabla(\nabla E)\\ \mathcal{R}\{\cdot\}=\mathbf{v}^{\mathrm{T}}\nabla$$

有$\mathcal{R}\{\mathbf{w}\}=\mathbf{v}$.

类似计算weight的gradient的forward和backward propagation可以计算所有

$$\begin{array}{l} \mathcal{R}\left\{\frac{\partial E}{\partial w_{k j}}\right\}=\mathcal{R}\left\{\delta_{k}\right\} z_{j}+\delta_{k} \mathcal{R}\left\{z_{j}\right\} \\ \mathcal{R}\left\{\frac{\partial E}{\partial w_{j i}}\right\}=x_{i} \mathcal{R}\left\{\delta_{j}\right\} \end{array}$$

即$\mathbf{v}^{\mathrm{T}}\mathbf{H}$的element.

5.5. Regularization in Neural Networks

Neural network的input size和output size是由dataset决定,而hidden layer的大小代表了model的complexity.一个重要的问题是如何balance between under-fit与over-fit.

5.5.1 Consistent Gaussian priors

最直接的加入regularizer:

$$\widetilde{E}(\mathbf{w})=E(\mathbf{w})+\frac{\lambda}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}$$

但这种方式破坏了consistent(假设input或者output经过线性变换,consistent的network是weight对应线性变换保持mapping function不变).这会导致network会favour某个解相比另一个等价解.

一种解决方式是给每层weight加入不同的regularizer:

$$\frac{\lambda_{1}}{2} \sum_{w \in \mathcal{W}_{1}} w^{2}+\frac{\lambda_{2}}{2} \sum_{w \in \mathcal{W}_{2}} w^{2}$$

即对应prior:

$$p\left(\mathbf{w} \mid \alpha_{1}, \alpha_{2}\right) \propto \exp \left(-\frac{\alpha_{1}}{2} \sum_{w \in \mathcal{W}_{1}} w^{2}-\frac{\alpha_{2}}{2} \sum_{w \in \mathcal{W}_{2}} w^{2}\right)$$

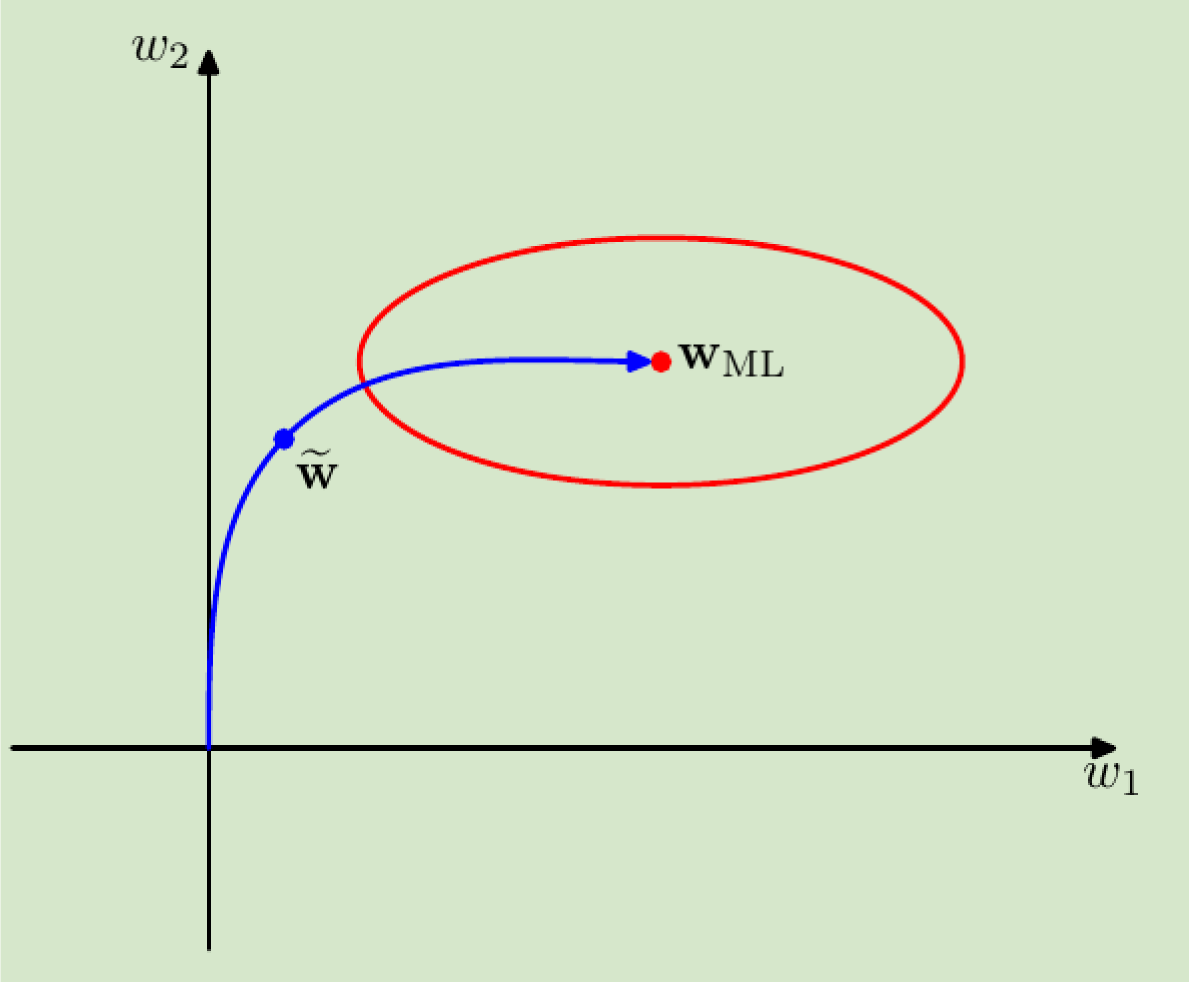
但是这种prior是improper的(由于bias parameter unconstrained,无法被normalize).

更general的做法是将parameter group起来,每个group有不同的prior:

$$\begin{array}{c} p(\mathbf{w}) \propto \exp \left(-\frac{1}{2} \sum_{k} \alpha_{k}\|\mathbf{w}\|_{k}^{2}\right) \\ \|\mathbf{w}\|_{k}^{2}=\sum_{j \in \mathcal{W}_{k}} w_{j}^{2} \end{array}$$

5.5.2 Early stopping

Early stopping 旨在只保留validation set中最低error下的model.这其实和regularization类似.$\tau\eta$扮演了regularization中λ的角色(τ是迭代次数,η是学习率).



类似于MAP的正则效果(MAP的先验体现在将最优的\tilde{w}往原点拉)

5.5.3 Invariances

许多application of neural network都需要一个property:**invariances**.例如handwriting digits recognize任务,当一张digit image作translate或rotation等一些变化后,得到的结果仍然是同一个数字.

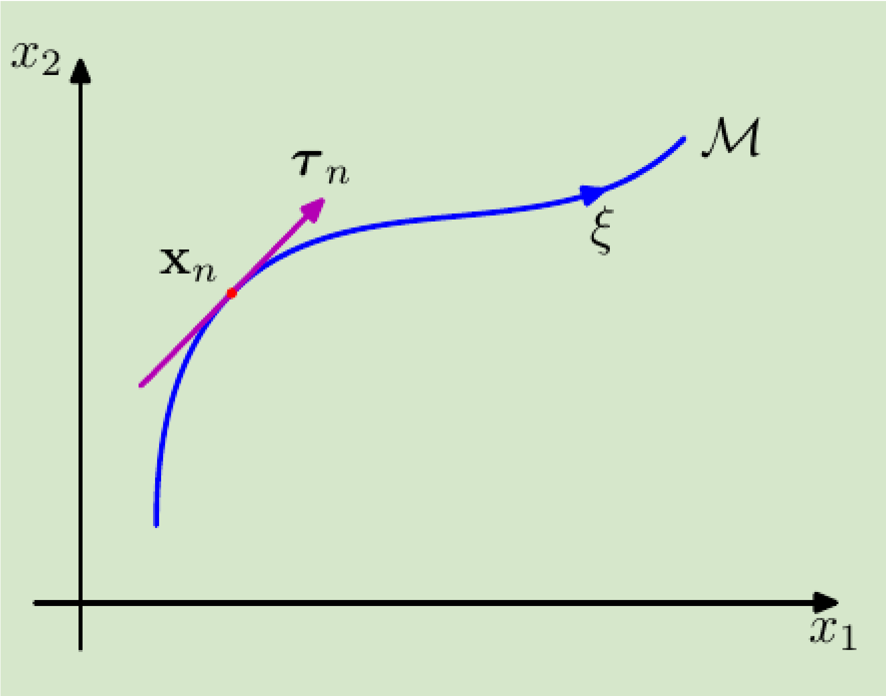
最直接的方法是提供足够多的data,让model去adaptive这种invariance.但实际中会受data limit,这就需要考虑其他的方法:

1. Data augument.人为在origin data上加入一些transform.
2. Regularization.当input发生一个transform后,penalize model output的change(*tangent propagation*)
3. Invariance feature prepossess.将model的input替换为hand-craft的invariance feature.(这对特征要求高,即要保留足够information去recognize,又要具有invariance的property)
4. Build a neural network with invariance property.

5.5.4 Tangent propagation

先做些简化假设:只考虑continuous transform(translate,rotation,not flip),transform只收一个parameter \xi.

当一个transform在\mathbf{x}上做一个连续不断的作用时,会得到一个input space上的一个manifold.



一个example,原始的input是x_n,transform会沿着$\mathcal{M}$产生新的$\mathbf{x}$,其中的$\boldsymbol{\tau}_n$是$\mathcal{M}$在$\mathbf{x}_n$上的tangent.

Tangent定义:

$$\boldsymbol{\tau}_{n}=\left.\frac{\partial \mathbf{s}\left(\mathbf{x}_{n}, \xi\right)}{\partial \xi}\right|_{\xi=0}$$

Model output关于这个transform的影响是:

$$\left.\frac{\partial y_{k}}{\partial \xi}\right|_{\xi=0}=\left.\sum_{i=1}^{D} \frac{\partial y_{k}}{\partial x_{i}} \frac{\partial x_{i}}{\partial \xi}\right|_{\xi=0}=\sum_{i=1}^{D} J_{k i} \tau_{i}$$

其中的$\mathbf{J}$是Jacobian matrix.这样就很自然的,对这个影响加上regularization就是增加model的invariance:

$$\Omega=\frac{1}{2} \sum_{n} \sum_{k}\left(\left.\frac{\partial y_{n k}}{\partial \xi}\right|_{\xi=0}\right)^{2}=\frac{1}{2} \sum_{n} \sum_{k}\left(\sum_{i=1}^{D} J_{n k i} \tau_{n i}\right)^{2}$$

5.5.5 Training with transformed data

其实等价于regularization的方法.

5.5.6 Convolutional networks

convolution network通过local receptive,weight share,subsampling实现invariance.
每层layer的unit以grid的形式排列.

5.5.7 Soft weight sharing

Convolution是对weight加入hard constrain,让每个group的weight相等.现在考虑让每个group的weight尽可能similar,这样可以增加network的表达能力.

之前在对network加入weight decay也就是加入了对weight的Gaussian prior.现在使用多个group的Gaussian prior,每个group都是一个Gaussian,那么所有weight的probability:

$$\begin{array}{c} p(\mathbf{w})=\prod_{i} p\left(w_{i}\right) \\ p\left(w_{i}\right)=\sum_{j=1}^{M} \pi_{j} \mathcal{N}\left(w_{i} \mid \mu_{j}, \sigma_{j}^{2}\right) \end{array}$$

取negative logarithm可以得出对应的regularization term:
$$\Omega(\mathbf{w})=-\sum_{i} \ln \left(\sum_{j=1}^{M} \pi_{j} \mathcal{N}\left(w_{i} \mid \mu_{j}, \sigma_{j}^{2}\right)\right) .$$

最终的error function变为:
$$\widetilde{E}(\mathbf{w})=E(\mathbf{w})+\lambda \Omega(\mathbf{w})$$

为了minimize整个error function,对所有未知的parameter求derivatives再利用optimization methods就能训练model.

5.6 Mixture Density Networks

之前谈过,SSE function就是基于Gaussian noise的假设,但是实际中很多model并不是基于Gaussian的,强行使用就会导致范化性很差.

我们因此寻找一个conditional probability output而不是简单的mean.这样的输出 $p(\mathbf{t}|\mathbf{x})$就能适用任意distribution的假设.

现在考虑使用mixture of Gaussian:

$$p(\mathbf{t} \mid \mathbf{x})=\sum_{k=1}^{K} \pi_{k}(\mathbf{x}) \mathcal{N}\left(\mathbf{t} \mid \boldsymbol{\mu}_{k}(\mathbf{x}), \sigma_{k}^{2}(\mathbf{x})\right)$$

所有未知参数都通过network的output来得到.其中的mixture coefficient满足:
$$\sum_{k=1}^{K} \pi_{k}(\mathbf{x})=1, \quad 0 \leqslant \pi_{k}(\mathbf{x}) \leqslant 1$$

这可以通过softmax的activation function实现.
error function为:
$$E(\mathbf{w})=-\sum_{n=1}^{N} \ln \left\{\sum_{k=1}^{k} \pi_{k}\left(\mathbf{x}_{n}, \mathbf{w}\right) \mathcal{N}\left(\mathbf{t}_{n} \mid \boldsymbol{\mu}_{k}\left(\mathbf{x}_{n}, \mathbf{w}\right), \sigma_{k}^{2}\left(\mathbf{x}_{n}, \mathbf{w}\right)\right)\right\}$$

只要对所有parameter微分并update,就能数值求解model.

5.7 Bayesian Neural Networks

1. 先利用prior和likelihood求出\mathbf{w}的MAP.
2. predictive function就可以写出解析形式.(由于network的非线性,用Laplace approximate)
3. 利用model evidence寻找最优hyper parameter(再次用到Laplace approximate)