9
Theory uncertainties

Markus Diehl

Exercise 9.1: The running QCD coupling

We want to compute the coefficient $a_3(\mu/Q)$ in the expansion

$$\alpha_s(Q) = \alpha_s(\mu) + a_1\Big(\frac{\mu}{Q}\Big)\,\alpha_s^2(\mu) + a_2\Big(\frac{\mu}{Q}\Big)\,\alpha_s^3(\mu) + a_3\Big(\frac{\mu}{Q}\Big)\,\alpha_s^4(\mu) + \mathcal{O}(\alpha_s^5)\,, \tag{9.1}$$

where we write μ instead of μ_R for simplicity, as we did in section 9.2.1.1. Following the derivation given there, we need the expression (9.7) of the β function to one order higher, i.e.

$$\begin{aligned}\beta\big(\alpha_s(Q)\big) &= -b_0\,\alpha_s^2(Q) - b_1\,\alpha_s^3(Q) - b_2\,\alpha_s^4(Q) + \mathcal{O}(\alpha_s^5)\\ &= -b_0\,\alpha_s^2(\mu) - 2a_1\Big(\frac{\mu}{Q}\Big)\,b_0\,\alpha_s^3(\mu) - \bigg[2a_2\Big(\frac{\mu}{Q}\Big) + a_1^2\Big(\frac{\mu}{Q}\Big)\bigg]\,b_0\,\alpha_s^4(\mu)\\ &\quad - b_1\,\alpha_s^3(\mu) - 3a_1\Big(\frac{\mu}{Q}\Big)\,b_1\,\alpha_s^4(\mu) - b_2\,\alpha_s^4(\mu) + \mathcal{O}(\alpha_s^5)\,.\end{aligned} \tag{9.2}$$

Differentiating of (9.1) with respect to $\ln Q^2$ gives the expression (9.2) on the left-hand-side and derivatives of $a_i(\mu/Q)$ on the right-hand-side. Matching the coefficients of $\alpha_s^4(\mu)$ leads to

$$\begin{aligned}\frac{\mathrm{d}a_3}{\mathrm{d}\ln Q^2} &= -\bigg[2a_2\Big(\frac{\mu}{Q}\Big) + a_1^2\Big(\frac{\mu}{Q}\Big)\bigg]\,b_0 - 3a_1\Big(\frac{\mu}{Q}\Big)\,b_1 - b_2\\ &= -3b_0^3\,L^2\Big(\frac{\mu}{Q}\Big) + 5b_0\,b_1\,L\Big(\frac{\mu}{Q}\Big) - b_2\end{aligned} \tag{9.3}$$

with $L(\mu/Q) = \ln(Q^2/\mu^2)$, where in the second step we have used our previous results (9.8) for $a_1(\mu/Q)$ and $a_2(\mu/Q)$. The differential equation (9.3) is readily solved and gives

$$a_3\Big(\frac{\mu}{Q}\Big) = -b_2\,L\Big(\frac{\mu}{Q}\Big) + \frac{5}{2}\,b_0\,b_1\,L^2\Big(\frac{\mu}{Q}\Big) - b_0^3\,L^3\Big(\frac{\mu}{Q}\Big)\,. \tag{9.4}$$

Let us compare the expansion (9.1) with the direct solution of the three-loop renormalisation group equation, $\mathrm{d}\alpha_s(Q)/\mathrm{d}\ln(Q^2) = -b_0\,\alpha_s^2(Q) - b_1\,\alpha_s^3(Q) - b_2\,\alpha_s^4(Q)$.

	m_t	$M_Z/2$	m_b
expansion (9.1) in $\alpha_s(\mu)$ with $\mu = M_Z$	0.1091	0.1323	0.2105
expansion (9.5) in $1/\ln(Q/\Lambda_{\text{QCD}})$	0.1091	0.1323	0.2255

Table 9.1 Values of the running coupling $\alpha_s(Q)$ obtained with either (9.1) or (9.5). In both cases, $\alpha_s(M_Z) = 0.1184$ is taken as input.

According to equation (6) in [1] we have

$$\alpha_s(Q) = \frac{1}{b_0 L'} - \frac{1}{(b_0 L')^2}\frac{b_1}{b_0}\ln L' + \frac{1}{(b_0 L')^3}\left[\frac{b_1^2}{b_0^2}\left(\ln^2 L' - \ln L' - 1\right) + \frac{b_2}{b_0}\right] \tag{9.5}$$

with $L' = \ln\left(Q^2/\Lambda_{\text{QCD}}^2\right)$. The relevant β function coefficients read [1]

$$b_0 = \frac{33 - 2n_F}{12\pi}\,, \quad b_1 = \frac{153 - 19n_F}{24\pi^2}\,, \quad b_2 = \frac{77139 - 15099n_F + 325n_F^2}{3456\pi^3}\,. \tag{9.6}$$

For the mass range considered in this exercise we have $n_f = 5$ active quark flavours, and the coefficients evaluate to

$$b_0 \approx 0.61\,, \qquad b_1 \approx 0.24\,, \qquad b_2 \approx 0.09\,. \tag{9.7}$$

We note that they nicely decrease in size, so that we expect good convergence of the expansion (9.2). In order to obtain $\alpha_s(M_Z) = 0.1184$ [1, 2] in (9.5), we need the value $\Lambda_{\text{QCD}} = 213$ MeV for the QCD scale parameter. For masses we use the values

$$m_b = 4.18 \text{ GeV}\,, \qquad m_t = 160 \text{ GeV}\,, \qquad M_Z = 91.1876 \text{ GeV} \tag{9.8}$$

from [2], where the quark masses m_q (with $q = b, t$) are running $\overline{\text{MS}}$ masses evaluated at the renormalisation scale $\mu_R = m_q$.

The results for the running coupling are given in table 9.1. We see that for $\mu = m_t$ and $\mu = M_Z/2$ the two representations (9.1) and (9.5) agree within the given accuracy. For $\mu = m_b$ there is, however, a discrepancy of about 7%. This indicates that the accuracy of the expansion (9.1) is degraded by powers of the large logarithm $L(M_Z/m_b) = \ln(m_b^2/M_Z^2) \approx -6.2$ in missing higher-order terms. In this situation, the direct solution (9.5) of the renormalisation group equation is more reliable.

Exercise 9.2: Perturbative expansion I

As in the previous exercise, we write μ instead of μ_R for simplicity. Acting with the derivative (9.24) in the book on the expansion (9.5) of C we obtain

$$\begin{aligned}\frac{\mathrm{d}C}{\mathrm{d}\ln\mu^2} &= \left[\frac{\partial}{\partial\ln\mu^2}C_1\left(\frac{\mu}{Q}\right)\right]\alpha_s^{k+1}(\mu) + \left[\frac{\partial}{\partial\ln\mu^2}C_2\left(\frac{\mu}{Q}\right)\right]\alpha_s^{k+2}(\mu)\\ &\quad - \left[b_0\,\alpha_s^2(\mu) + b_1\,\alpha_s^3(\mu)\right]\left[C_0\,k\alpha_s^{k-1}(\mu) + C_1\left(\frac{\mu}{Q}\right)(k+1)\,\alpha_s^k(\mu)\right] + \mathcal{O}(\alpha_s^{k+3})\,,\end{aligned} \tag{9.9}$$

where we have used the perturbative expansion (9.4) of the β function. With the explicit expressions for $C_1(\mu/Q)$ and $C_2(\mu/Q)$ in (9.9) we find

$$\begin{aligned}\frac{\mathrm{d}C}{\mathrm{d}\ln\mu^2} &= k\,b_0\,C_0\,\alpha_s^{k+1}(\mu)\\ &\quad + \left\{(k+1)\,b_0\,C_1(1) + k\,b_1\,C_0 - k(k+1)\,b_0^2\,C_0\,L\left(\frac{\mu}{Q}\right)\right\}\alpha_s^{k+2}(\mu)\\ &\quad - b_0\,C_0\,k\,\alpha_s^{k+1} - b_1\,C_0\,k\,\alpha_s^{k+2}\\ &\quad - b_0\left\{C_1(1) - k\,b_0 C_0\,L\left(\frac{\mu}{Q}\right)\right\}(k+1)\,\alpha_s^{k+2}(\mu) + \mathcal{O}(\alpha_s^{k+3})\\ &= \mathcal{O}(\alpha_s^{k+3})\,,\end{aligned} \tag{9.10}$$

where $L(\mu/Q) = \ln(Q^2/\mu^2)$ and hence $\partial L(\mu/Q)\big/\partial\ln\mu^2 = -1$.

Exercise 9.3: Perturbative expansion II

Inserting the expansion (9.14) into (9.13) we obtain

$$\begin{aligned}&\left[\frac{\partial}{\partial\ln\mu_F^2}\,C_1\left(\frac{\mu_F}{Q},\frac{\mu_R}{Q}\right)\right]\alpha_s^{k+1}(\mu_R) + \left[\frac{\partial}{\partial\ln\mu_F^2}\,C_2\left(\frac{\mu_F}{Q},\frac{\mu_R}{Q}\right)\right]\alpha_s^{k+2}(\mu_R) + \mathcal{O}(\alpha_s^{k+3})\\ &= -P\big(\alpha_s(\mu_F)\big)\otimes\left\{C_0\,\alpha_s^k(\mu_R) + C_1\left(\frac{\mu_F}{Q}.\frac{\mu_R}{Q}\right)\alpha_s^{k+1}(\mu_R)\right\} + \mathcal{O}(\alpha_s^{k+3})\,.\end{aligned} \tag{9.11}$$

To match the accuracy of the left-hand-side, we must expand $P\big(\alpha_s(\mu_F)\big)$ in $\alpha_s(\mu_R)$ up to second order. Using (9.6) and (9.8) in (9.12), we have

$$P\big(\alpha_s(\mu_F)\big) = P_0\left[\alpha_s(\mu_R) - b_0\ln\frac{\mu_F^2}{\mu_R^2}\,\alpha_s^2(\mu_R)\right] + P_1\,\alpha_s^2(\mu_R) + \mathcal{O}(\alpha_s^3)\,, \tag{9.12}$$

so that the right-hand-side of (9.11) turns into

$$
\begin{aligned}
&- P_0 \otimes C_0 \left[\alpha_s^{k+1}(\mu_R) - b_0 \ln \frac{\mu_F^2}{\mu_R^2} \, \alpha_s^{k+2}(\mu_R) \right] \\
&\qquad - P_0 \otimes C_1 \left(\frac{\mu_F}{Q} \cdot \frac{\mu_R}{Q} \right) \alpha_s^{k+2}(\mu_R) - P_1 \otimes C_0 \, \alpha_s^{k+2}(\mu_R) + \mathcal{O}(\alpha_s^{k+3}) \, .
\end{aligned}
\tag{9.13}
$$

Comparing this with the left-hand-side of (9.11) gives

$$
\frac{\partial}{\partial \ln \mu_F^2} \, C_1\left(\frac{\mu_F}{Q}, \frac{\mu_R}{Q} \right) = -P_0 \otimes C_0 \tag{9.14}
$$

$$
\Rightarrow \quad C_1\left(\frac{\mu_F}{Q}, \frac{\mu_R}{Q} \right) = C_1\left(1, \frac{\mu_R}{Q} \right) + P_0 \otimes C_0 \ln \frac{Q^2}{\mu_F^2} \tag{9.15}
$$

and

$$
\begin{aligned}
\frac{\partial}{\partial \ln \mu_F^2} \, C_2\left(\frac{\mu_F}{Q}, \frac{\mu_R}{Q} \right) &= -P_1 \otimes C_0 - P_0 \otimes C_1\left(1, \frac{\mu_R}{Q} \right) \\
&\quad + P_0 \otimes P_0 \otimes C_0 \ln \frac{\mu_F^2}{Q^2} + b_0 \, P_0 \otimes C_0 \left(\ln \frac{\mu_F^2}{Q^2} + \ln \frac{Q^2}{\mu_R^2} \right)
\end{aligned}
\tag{9.16}
$$

$$
\begin{aligned}
\Rightarrow \quad C_2\left(\frac{\mu_F}{Q}, \frac{\mu_R}{Q} \right) &= C_2\left(1, \frac{\mu_R}{Q} \right) \\
&\quad + \left[P_1 \otimes C_0 + P_0 \otimes C_1\left(1, \frac{\mu_R}{Q} \right) - b_0 \, P_0 \otimes C_0 \, \ln \frac{Q^2}{\mu_R^2} \right] \ln \frac{Q^2}{\mu_F^2} \\
&\quad + \frac{1}{2} \Big[b_0 \, P_0 \otimes C_0 + P_0 \otimes P_0 \otimes C_0 \Big] \ln^2 \frac{Q^2}{\mu_F^2} \, ,
\end{aligned}
\tag{9.17}
$$

where in the differential equation (9.16) we have already inserted the solution (9.15). If we use (9.9) to make the μ_R dependence explicit, we obtain

$$
\begin{aligned}
C_1\left(\frac{\mu_F}{Q}, \frac{\mu_R}{Q} \right) &= C_1(1,1) + P_0 \otimes C_0 \, \ln \frac{Q^2}{\mu_F^2} - k \, b_0 \, C_0 \, \ln \frac{Q^2}{\mu_R^2} \, , \\
C_2\left(\frac{\mu_F}{Q}, \frac{\mu_R}{Q} \right) &= C_2(1,1) + \Big[P_1 \otimes C_0 + P_0 \otimes C_1(1,1) \Big] \ln \frac{Q^2}{\mu_F^2} \\
&\quad - \Big[k \, b_1 \, C_0 + (k+1) \, b_0 \, C_1(1,1) \Big] \ln \frac{Q^2}{\mu_R^2} \\
&\quad + \frac{1}{2} \Big[b_0 \, P_0 \otimes C_0 + P_0 \otimes P_0 \otimes C_0 \Big] \ln^2 \frac{Q^2}{\mu_F^2} + \frac{k(k+1)}{2} \, b_0^2 \, C_0 \, \ln^2 \frac{Q^2}{\mu_R^2} \\
&\quad - (k+1) \, b_0 \, P_0 \otimes C_0 \, \ln \frac{Q^2}{\mu_F^2} \, \ln \frac{Q^2}{\mu_R^2} \, .
\end{aligned}
\tag{9.18}
$$

We see that C_i is a polynomial of order i in the two logarithms $\ln(Q^2/\mu_F^2)$ and $\ln(Q^2/\mu_R^2)$.

Exercise 9.4: Evolution equations
Recursive application of the definition

$$[f \otimes g](x) = \int_x^1 \frac{\mathrm{d}z}{z}\, f(z)\, g\Big(\frac{x}{z}\Big) \tag{9.19}$$

gives

$$\big[(f \otimes g) \otimes h\big](x) = \int_x^1 \frac{\mathrm{d}y}{y} \int_y^1 \frac{\mathrm{d}z}{z}\, f(z)\, g\Big(\frac{y}{z}\Big)\, h\Big(\frac{x}{y}\Big) \tag{9.20}$$

and

$$\begin{aligned}\big[f \otimes (g \otimes h)\big](x) &= \int_x^1 \frac{\mathrm{d}z}{z}\, f(z) \int_{x/z}^1 \frac{\mathrm{d}v}{v}\, g(v)\, h\Big(\frac{x}{vz}\Big)\\ &= \int_x^1 \frac{\mathrm{d}z}{z} \int_x^z \frac{\mathrm{d}y}{y}\, f(z)\, g\Big(\frac{y}{z}\Big)\, h\Big(\frac{x}{y}\Big)\,,\end{aligned} \tag{9.21}$$

where in the last step we have made the substitution $y = vz$. Noting that the integrals $\int_x^1 \mathrm{d}y \int_y^1 \mathrm{d}z$ and $\int_x^1 \mathrm{d}z \int_x^z \mathrm{d}y$ are both over the region $x < y < z < 1$, we see that (9.20) and (9.21) are equal.

Exercise 9.5: Renormalisation scale variation
The curves in Figure 9.4 in the book (reproduced here as Figure 9.1) correspond to the following values and errors of Γ (given in units of keV):

	LO	NLO	NNLO	NNNLO
$\mu = M_H$	166^{+37}_{-28}	272^{+36}_{-32}	305^{+11}_{-17}	$308^{+0.4}_{-5}$
$\mu = M_H/2$	203^{+51}_{-37}	308^{+38}_{-36}	316^{+1}_{-11}	307^{+2}_{-8}

The strongly asymmetric error of the NNLO value for $\mu = M_H/2$ arises because the corresponding curve has a shallow maximum at $\mu \approx 0.4\,M_H$. Notice that to correctly determine the corresponding error, one needs Γ in the full interval $\frac{1}{2}M_H \le \mu \le 2M_H$ and not just at the end points $\mu = \frac{1}{2}M_H$ and $\mu = 2M_H$. In a similar fashion, the strongly asymmetric errors of the NNLO values (for both choices of the central scale) are due to a shallow maximum of the corresponding curve at $\mu \approx 0.8\,M_H$.

A graphical representation of the values and errors is given in figure 9.2. We see features that are typical of observables whose tree-level value depends on a high power of α_s. There is a rather large shift from the values at LO to those at NLO — larger than suggested by the uncertainty estimate based on scale variation by a factor between $\frac{1}{2}$ to 2. As one goes to even higher orders, the changes in central values become milder, as well as the dependence on the choice of μ.

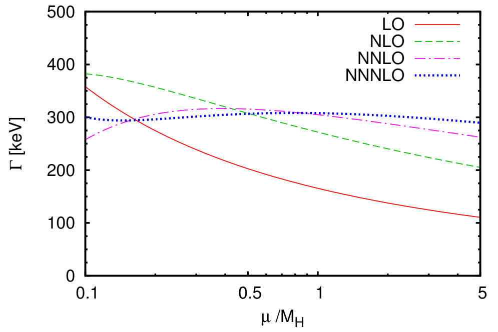

Figure 9.1 (corresponds to figure 9.4 in the book) The partial width Γ for Higgs-boson decay into hadrons via a top-quark loop, calculated at successive orders in α_s and plotted as a function of the renormalisation scale μ in units of M_H. Parameters used are the pole masses $M_H = $ 120 GeV and $m_t = $ 175 GeV. The running coupling is taken at the same perturbative order as the observable, with $\alpha_s(M_Z) = 0.1184$ in all cases.

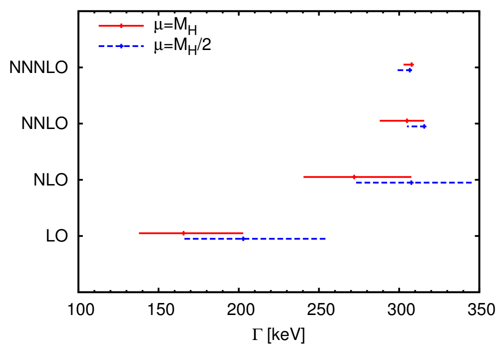

Figure 9.2 Values of Γ corresponding to the curves in figure 9.1. The error bars correspond to a scale variation by a factor between $\frac{1}{2}$ to 2 around the central scale.

Exercise 9.6: Lagrange multipliers and Hessian method

As stated below (9.22), we assume that the observable

$$F(\mathbf{p}) = F(\mathbf{p}_{\text{min}}) + \mathbf{D}^T \cdot (\mathbf{p} - \mathbf{p}_{\text{min}}) \tag{9.22}$$

is strictly linear and

$$\Delta\chi^2(\mathbf{p}) = \chi^2(\mathbf{p}) - \chi^2_{\text{min}} = (\mathbf{p} - \mathbf{p}_{\text{min}})^T \cdot H \cdot (\mathbf{p} - \mathbf{p}_{\text{min}}) \tag{9.23}$$

is strictly quadratic in the vector $\mathbf{p}$ of fit parameters. Here $\mathbf{D}$ is a fixed vector and H is the Hesse matrix, which is symmetric. To minimise $\chi^2(\mathbf{p})$ under the constraint $F(\mathbf{p}) = v$ we use the method of Lagrange multipliers and thus have to determine the stationary point of the function

$$\begin{aligned}\Lambda(\mathbf{p}, \lambda) &= \chi^2(\mathbf{p}) - \lambda\big[F(\mathbf{p}) - v\big] \\ &= \chi^2_{\text{min}} - \lambda\big[F(\mathbf{p}_{\text{min}}) - v\big] - \lambda \mathbf{D}^T \cdot (\mathbf{p} - \mathbf{p}_{\text{min}}) + (\mathbf{p} - \mathbf{p}_{\text{min}})^T \cdot H \cdot (\mathbf{p} - \mathbf{p}_{\text{min}})\,.\end{aligned} \tag{9.24}$$

This provides the conditions

$$\frac{\partial\Lambda(\mathbf{p}, \lambda)}{\partial\mathbf{p}} = 2H \cdot (\mathbf{p} - \mathbf{p}_{\text{min}}) - \lambda\mathbf{D} = 0 \qquad \Rightarrow \qquad \mathbf{p} - \mathbf{p}_{\text{min}} = \frac{\lambda}{2} H^{-1} \cdot \mathbf{D} \tag{9.25}$$

and

$$\frac{\partial\Lambda(\mathbf{p}, \lambda)}{\partial\lambda} = v - F(\mathbf{p}_{\text{min}}) - \mathbf{D}^T \cdot (\mathbf{p} - \mathbf{p}_{\text{min}}) = 0 \qquad \Rightarrow \quad v - F(\mathbf{p}_{\text{min}}) = \frac{\lambda}{2} \mathbf{D}^T \cdot H^{-1} \cdot \mathbf{D}\,, \tag{9.26}$$

which together fix $\mathbf{p}$ and λ. In the second step of (9.26) we have used the expression of $\mathbf{p} - \mathbf{p}_{\text{min}}$ derived in (9.25). Inserting the same expression in (9.23), we obtain

$$\chi^2_{\text{min}}\big|_{F=v} - \chi^2_{\text{min}} = \frac{\lambda^2}{4} \mathbf{D}^T \cdot (H^{-1})^T \cdot H \cdot H^{-1} \cdot \mathbf{D} = \frac{\lambda^2}{4} \mathbf{D}^T \cdot H^{-1} \cdot \mathbf{D} \tag{9.27}$$

for the value of $\chi^2(\mathbf{p})$ at the constrained minimum. We can finally use (9.26) to replace λ and then have

$$\chi^2_{\text{min}}\big|_{F=v} - \chi^2_{\text{min}} = \frac{\big[v - F(\mathbf{p}_{\text{min}})\big]^2}{\mathbf{D}^T \cdot H^{-1} \cdot \mathbf{D}}\,. \tag{9.28}$$

We see that $\chi^2_{\text{min}}\big|_{F=v}$ is quadratic in $\mathbf{v}$, as stated after (9.22). The condition (9.22) reads

$$\chi^2_{\text{min}}\big|_{F=v} - \chi^2_{\text{min}} = T^2\,, \tag{9.29}$$

where T is the tolerance, which according to (9.28) implies

$$v - F(\mathbf{p}_{\text{min}}) = \pm T \sqrt{\mathbf{D}^T \cdot H^{-1} \cdot \mathbf{D}}\,. \tag{9.30}$$

The two corresponding values of v determine the uncertainty on $F(\mathbf{p}_{\text{min}})$ in the Lagrange multiplier method. This is equivalent to the uncertainty computed in the Hessian method, which according to (9.19) reads

$$\Delta F = T\sqrt{\left(\frac{\partial F}{\partial \mathbf{p}}\right)^T H^{-1}\left(\frac{\partial F}{\partial \mathbf{p}}\right)} = T\sqrt{\mathbf{D}^T \cdot H^{-1} \cdot \mathbf{D}}\,, \tag{9.31}$$

where in the second step we have used (9.22).

Bibliography

1 S. Bethke, Eur. Phys. J. C **64** (2009) 689 [arXiv:0908.1135 [hep-ph]].

2 J. Beringer *et al.* [Particle Data Group Collaboration], Phys. Rev. D **86** (2012) 010001.